

Vortex-pair unbinding in the normal state of two-dimensional, short coherence-length superconductors

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We study the superconducting transition in the attractive Hubbard model in two dimensions using the self-consistent T -matrix approximation. We demonstrate that for large system sizes, this approximate method produces XY critical scaling in the correlation length and pair susceptibility. For the parameters we investigate, the critical regime is quite large, extending beyond 5 times T_{KTB} . We discuss the role of vortex-pair unbinding in the normal state in the context of pseudogap behaviour and the relevance to the physics of underdoped cuprates.

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Compared to conventional superconductors, the ratio of the superconducting pair wave-function size to the average inter-carrier spacing is many orders of magnitude lower in the cuprates. Consequently, the pairing in the cuprates is much less mean-field like and quite some time ago it was argued [1] that, in the cuprates, strong pairing correlations should modify the normal state behaviour between the transition temperature T_c and the mean-field transition temperature T^* . Early evidence for this pre-cursor pairing was the comparison between numerical simulations [2] of the attractive Hubbard model with the suppression of the Knight shift and nuclear relaxation rate [3] between T_c and room temperature in underdoped YBCO. The body of experimental evidence for pre-cursor pairing in underdoped cuprates has grown considerably, for instance, optical conductivity [4] and specific heat [5] experiments also indicate a loss of weight for normal state carriers between T_c and T^* . These measurements, involve thermodynamics or two-particle response and are insensitive to the symmetry of the pairing. The recent angle-resolved photo-emission (ARPES) results [6,7] have now confirmed this picture of a loss of single-particle spectral weight in the normal state, and in addition, have confirmed a symmetry consistent with $d_{x^2-y^2}$ -pairing.

Staring from the notion that improved understanding of the cuprates requires theories of much stronger pairing than we are used to, one is naturally lead to generalizations of BCS theory. Arguably the simplest candidate for such theories is the attractive Hubbard model which incorporates increased fluctuations due to reduced dimensionality with strong (albeit s -wave) pairing and the possibility of small pair sizes. Studies of this model have generally focussed on either the phase diagram or the unusual normal state. Moreo and Scalapino [8] followed on earlier work by Scalettar et al [9] to estimate the ordering temperature by performing finite-size scaling on the pair susceptibility. Their Monte Carlo (MC) simulations on systems up to size 10×10 gave $T_{KTB} \approx 0.045$ for $U = -4$ at quarter-filling (density $n = 0.5$, energy in units of t). Subsequently, Assad et al [10] investigated the onset of a non-zero superfluid stiffness ρ_s using MC simulations on systems of size 8×8 . Very recently, Deisz et al [11] used the fluctuation-exchange approximation [12] (FEA) to study the superfluid stiffness and the entropy. Most of their data was on significantly larger 32×32 systems and their FEA results agree well with the MC data. However,

they observe a broad onset of $\rho_s(T)$ (that does not scale as expected with system size) instead of the discontinuity of the KTB transition. [13] The dilemma is that without a better understanding of the correlation length it is difficult to disentangle finite-size effects, and spurious long-range order from the expected algebraic order.

The other class of studies, originated with the MC calculations of Randeria et al [2] of the temperature dependence of the spin susceptibility $\chi_{\text{spin}}(T)$, the nuclear relaxation rate $T_1(T)$ and the density of states at the Fermi surface $N_0(T)$. Their results agreed qualitatively with experiments on underdoped cuprates and at an early stage suggested that precursor pairing is manifested in the normal state of these materials. Further investigations in this vein included the MC simulations of Singer et al [14] who calculated the frequency dependence of the density of states $N(\omega)$. In addition to the potentially exact MC calculations our earlier gaussian fluctuation studies [1,15] were extended to the self-consistent T -matrix approximation [16] (STA) which although approximate, allows for the study of different hamiltonians and larger systems. From a diagrammatic point of view, the STA includes a subset of the diagrams in the FEA. Using this self-consistent T -matrix approximation we recently investigated [17] pre-cursor pairing in a model with d -wave symmetry that led to very interesting predictions tested in recent ARPES experiments. [18]

Our goal in this paper is to study the critical behaviour of the attractive Hubbard model in the parameter range relevant for the cuprates, and investigate any connections between the Kosterlitz-Thouless-Berezinskii (KTB) transition and the anomalous normal state properties. We demonstrate that the self-consistent T -matrix approximation is sufficiently accurate to produce XY critical scaling in the correlation length and pair susceptibility. The model has a large critical regime with $\xi(T)$ falling off exponentially from T_{KTB} until $\xi \sim 1$ (in units of the lattice spacing). This happens somewhat before T^* and above this temperature the pre-cursor pairs are essentially uncorrelated. Given that the STA includes a subset of the FEA diagrams we conclude that both these approximations capture the delicate interplay [19] between the carriers, the precursor pairs and the unpairing of vortices.

The attractive Hubbard model hamiltonian is

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + hc) - |U| \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where the first sum runs over pairs of nearest neighbour sites on a two-dimensional (2D) square lattice. By varying the attraction U one can study the crossover from BCS superconductivity in weak coupling, to the Bose condensation of local pairs in strong coupling. In 2D, the broken $U(1)$ symmetry belongs to the XY universality class and one expects a KTB-type transition at non-zero temperature. On the other hand, at half-filling, superconductivity becomes degenerate with a charge-density-wave instability, and this larger $SU(2)$ symmetry requires the ordering temperature to vanish.

We study this model by self-consistently solving for the dressed propagator and four-point vertex. The Green's function is defined in terms of the self-energy $G(\mathbf{k}, ik_n) = [ik_n - \epsilon(k) + \mu - \Sigma(\mathbf{k}, ik_n)]^{-1}$. The exact self-energy is formally defined through the coupled equations

$$\Sigma(k) = U \sum G(q-k)G(p)G(q-p)\Gamma_{p,k}(q) \quad (2)$$

and

$$\Gamma_{k,k'}(q) = I_{k,k'}(q) - \sum I_{k,p}(q)G(p)G(q-p)\Gamma_{p,k'}(q) \quad (3)$$

where the sum (with proper factors) represents a trace over intermediate momenta, frequencies and, where appropriate, spins. Here $I_{k,k'}(q)$ is the irreducible particle-particle vertex, $k = (\mathbf{k}, ik_n)$ and $q = (\mathbf{q}, iq_n)$ in a temperature formalism with Fermi and Bose Matsubara frequencies $k_n = (2n+1)\pi T$ and $q_n = 2n\pi T$ respectively. Determining the full irreducible particle-particle vertex is a formidable task and we approximate $I_{k,k'}(q)$ by the bare Hubbard potential. Our description then reduces to the self-consistent T -matrix approximation. Now $\Gamma_{k,k'}(q) = \Gamma(q)$ and (3) simplifies to the separable Bethe-Salpeter equation with solution

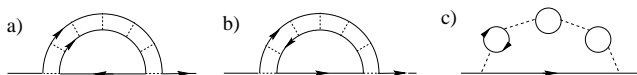
$$\Gamma(q) = \frac{U^2 \Pi(q)}{1 + U \Pi(q)} \quad (4)$$

and (2) reduces to

$$\Sigma(k) = \sum_q G(q-k)\Gamma(q). \quad (5)$$

We have subtracted the Hartree shift and the particle-particle bubble $\Pi(q) = \sum_k G(q-k)G(k)$ is defined in terms of dressed propagators.

This amounts to keeping the subset of particle-particle diagrams in the fluctuation exchange approximation. The self-energy in the FEA includes diagrams in three channels



while we only keep the particle-particle channel represented by the first term. Our results confirm that this first class of diagrams are relevant and the particle-particle contributions are sufficient [19] to produce the correct critical behaviour for the densities we investigate. At half-filling neither the STA or the FEA methods preserve the degeneracy between pairing and CDW channels that is required to restore the full $SU(2)$ symmetry.

However, our calculations are sufficiently far from half-filling, such that this is not an issue. In fact, our STA results agree quite well with the Monte Carlo simulations [2], yielding a suppression of the density of states at the Fermi level that tracks the reduction of spin susceptibility similar to the Knight shift experiments. A more detailed comparison with MC will be presented elsewhere. [20]

Our goal here is to elucidate the nature of the normal state pairing correlations. Specifically we wish to investigate the equal-time pair correlation function

$$\Phi(\mathbf{r}) = \langle \bar{\Delta}(0,0)\Delta(\mathbf{r},0) \rangle. \quad (6)$$

This is the Fourier transform of the generalized pair susceptibility, which in our approximation has the simple form $\chi_{\text{pair}}(q) = \Pi(q)/[1 + U\Pi(q)]$.

To evaluate $\chi_{\text{pair}}(q)$, we employ the standard STA/FEA procedure of iteratively solving for (4) and (5) on an $L \times L$ lattice using fast Fourier transforms. We typically keep 256 Matsubara frequencies and to avoid finite-size effects study systems of size $L = 128$. Since this procedure uses periodic boundary conditions in space, $\Phi(r)$ only exhibits bulk character up to distance $r \sim L/2$. In Figure 1 we show our results for $\Phi(r)$ at four temperatures for $U = -4$ at quarter-filling. We use these parameters for comparison with the MC data [2] which show a reduction of the spin susceptibility below $T = 0.5$. The correlation function indeed decays exponentially and at large distances shows a very rapid increase upon cooling.

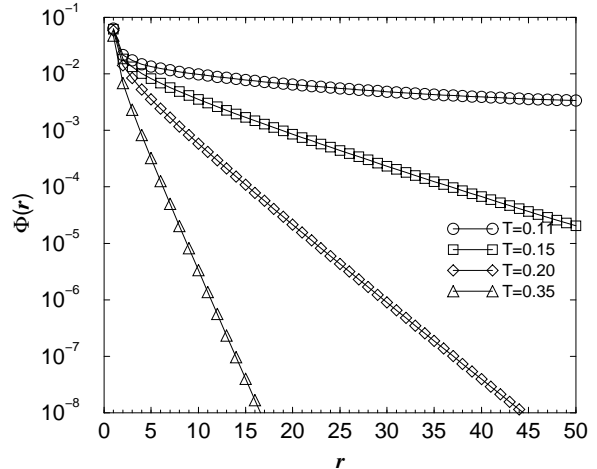


FIG. 1. Equal-time pair correlation function $\Phi(r)$ vs. position $r = |(x,0)|$ in units of the lattice spacing for $U = -4$, at quarter-filling, and temperatures $T = 0.35, 0.20, 0.15$ and 0.11 .

The correlation length ξ at each temperature is defined through the scaling relation [13]

$$\Phi(r) \sim \frac{1}{r^\eta} \times e^{-r/\xi}. \quad (7)$$

at large distances. To extract $\xi(T)$, the power law correction is small and can be neglected. (For the XY universality class the exponent has the theoretical value $\eta = 0.25$ which indeed is verified below). The temperature-dependence of $\xi(T)$ for the same attraction and density

is given as the circles in Figure 2. The solid line is a fit to the XY scaling form [13]

$$\xi(T) \sim \exp\left(\frac{A}{\sqrt{\beta_c - \beta}}\right) \quad (8)$$

with $\beta = 1/T$ the inverse temperature and $\beta_c = 1/T_{KTB}$ the inverse of the KTB transition temperature. The best fit yields $T_{KTB} = 0.049(2)$ for $U = -4$ and $n = 0.5$. For comparison we also show the power scaling law forms $\xi \sim (T - T_c)^{-\nu}$ for mean-field and 3D XY exponents $\nu = \frac{1}{2}$ and $\nu = \frac{2}{3}$ respectively.

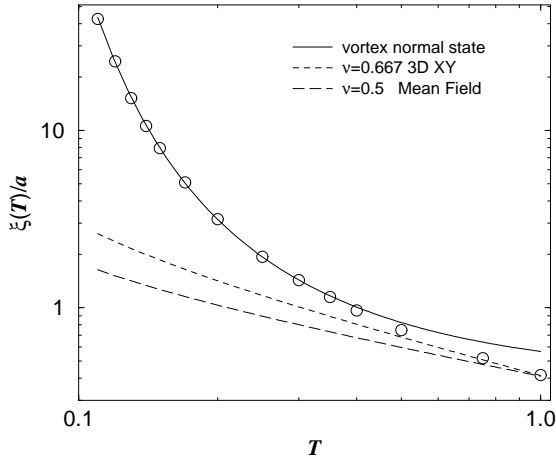


FIG. 2. Pair correlation length $\xi(T)$ vs. temperature T for $U = -4$, at quarter-filling. The solid line is a fit for the exponential XY scaling form. The broken and dash lines represent power-law scaling for the mean-field and 3D XY exponents $\nu = \frac{1}{2}$ and $\frac{2}{3}$.

The correlation length clearly scales according to the XY critical scaling form and upon heating decreases much faster than any power law. It is clearly natural to interpret this scaling as due to *vortex-pair unbinding* in normal state.

Furthermore, the numeric data shows critical scaling over a very large critical regime, from $T_{KTB} \approx 0.05$ up to $T \approx 0.30$. In fact, we observe critical scaling until the correlation length has decayed all the way down to a single lattice spacing! The MC simulations and our STA results show the suppression of the spin susceptibility starts to develop below $T \approx 0.5$. Since ξ does not exceed one lattice spacing in the temperature range $0.35 < T < 0.5$ we argue that to describe the onset of the pseudogap behaviour one needs to incorporate amplitude fluctuations in addition to phase fluctuations. The size of the critical regime is maximal (in the sense that it extends down to $\xi = 1$ in units of the lattice spacing) and the very large scaling regime is reminiscent of the quantum critical point. [21]

A further test for XY scaling is to consider the uniform, static, pair susceptibility which, in our approximation, is proportional to $\Gamma(q)$ with $q = 0$ in Eq. 4. Thus χ_{pair} diverges as $\lambda = -U\Pi(0) \rightarrow 1$. While λ reaches the value one at a non-zero temperature in mean-field theory, more accurate calculations such as MC, FEA or STA should never give $\lambda = 1$ for a finite system. In-

deed, our calculations agree with the FEA calculation of Ref. [11] yielding $\lambda < 1$ for *all* temperatures. In fact, this even holds in three dimensions clearly due to the absence of phase transitions in finite systems. However, provided we keep the system size $L > \xi(T)$, we can observe the approach to the divergence in χ_{pair} as T_{KTB} is approached from above. In Figure 3 we plot $\chi_{\text{pair}}(T)$ vs the temperature-dependent correlation length $\xi(T)$ to the power $2 - \eta$ for $U = -4$ and $n = 0.5$ at several temperatures.

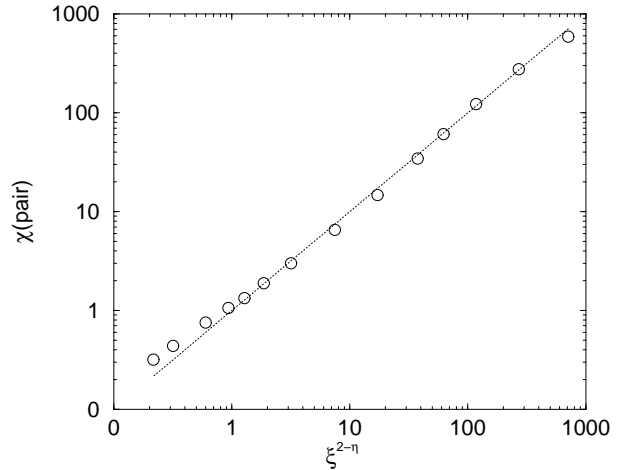


FIG. 3. Pair susceptibility $\chi_{\text{pair}}(T)$ vs. power-law scaling of the pair correlation length $\xi(T)^{2-\eta}$ for $\eta = \frac{1}{4}$.

We have explicitly set $\eta = \frac{1}{4}$ – the universal XY value. A fit to the lower temperature data gave $\eta \approx 0.248$. The error in χ_{pair} is larger due to the denominator of (4) as $\lambda \approx 1$ at low temperatures. None the less, our data shows XY critical scaling over nearly three orders of magnitude.

The degree to which both $\xi(T)$ and χ_{pair} displays XY scaling is remarkable. This demonstrates that the self-consistent T -matrix approximation which includes self-energy corrections but neglects vertex corrections still captures [19] the ‘relevant’ fluctuations. Further, the very large critical regime in the attractive Hubbard Model vindicates our assertion of the importance of small distance physics (which is neglected in low-energy, long-wavelength expansions).

We have been maintaining for some time [1,2,22] that as a model of a 2D short coherence length superconductors, the unusual normal state properties of the attractive Hubbard Model is of relevance to the high- T_c superconductors. This is especially true for the underdoped cuprates which are much more [23] two-dimensional than their optimally-doped or overdoped counterparts.

It is therefore natural to conclude that our results have far-reaching implications for the cuprates. The picture that emerges is that upon cooling the normal state behaviour is strongly influenced by the 2D XY critical point over a large temperature range, until three-dimensional coherence starts to develop just above the observed (3D) critical temperature. Thus, the strong 2D pairing correlations imply that (zero-field [24]) vortex-pair unbinding is important in the normal state of the cuprates and that vortices provide an additional (strong) scattering mech-

anism. This scattering channel disappears below T_c and although this s -wave model of course does not contain the d -wave pairing observed in ARPES experiments, this framework is clearly consistent with the observation of broad spectral peaks in the normal state which sharpen dramatically below T_c . The short distance over which phase-coherence is established then also explain why very strong paraconductivity is not observed over a large temperature range.

These results also emphasize that in order to study the onset of order numerically, one needs very large systems to eliminate finite size effects. The transition observed by Deisz et al [11] is therefore indeed a KTB type transition although the 32×32 systems they focussed on may be on the borderline of being influenced by finite-size effects. Whereas the STA/FEA methods may have problems near half-filling where the model has $SU(2)$ symmetry, these methods are very successful at keeping track of relevant pairing correlations away from half-filling while ensuring that large correlation lengths do not mimic spurious long-range order. These methods should therefore be used in studying a variety of models to complement the MC calculations which are restricted to smaller lattices, but of course have other advantages.

It should be noted that several other groups have emphasized 2D pair correlations in the cuprates, dating back to Uemura's [25] investigation of the superfluid density. Also, the physics we discuss here and introduced in Refs. [1,2,22,17] bears some resemblance to the framework developed later by Emery and Kivelson [26] – although they emphasize the proximity of an insulating state in the cuprates. The attractive Hubbard model is, however, also susceptible to a metal-insulator-transition near half-filling due to the charge-density-wave correlations, although this simple model may not capture the doped Mott insulator physics of the cuprates.

Above we have demonstrated the connection between XY fluctuations and pseudogap physics. It is important to emphasize that it is crucial to also be in the intermediate coupling (short coherence length) regime of the phase diagram. In the weak coupling limit XY fluctuations do not produce pseudogap behaviour over an appreciable temperature range. [27]

To summarize we have demonstrated that the self-consistent T -matrix approximation can capture the normal state XY physics of the unbinding of vortex pairs for the attractive Hubbard model in 2D. The scaling regime is very large, extending beyond 5 times T_{KTB} , until the correlation length has decreased down to a single lattice spacing. The large regime influenced by vortex-pair unbinding suggests that the excitations may be relevant to the normal state pseudogap behaviour of underdoped cuprates. The large window of temperatures where $\xi(T) \gg 10$ also implies that when investigating the development of order, it is important to complement MC calculations with STA/FEA calculations on large systems.

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